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Theoretical Studies and Modeling of III-V Nitride Materials and Devices for Optoelectronic Applications

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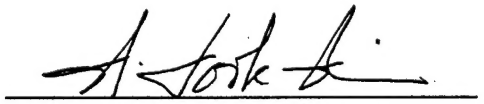

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13. ABSTRACT (Maximum 200 words)

Two main objectives of this research program include: (1) investigation of the fundamental material, transport, and optical properties of IIi-V nitrides; and (2) simulation and design optimization of GaN-based optoelectronic devices. Study of fundamental physical properties (such as carrier scattering and optical transitions) is based on an envelope function formalism for accurate description of band spectrum in bulk and confined structures. Numerical analyses and optimization of GaN-based devices are approached by solving a set of coupled equations self-consistently. This research initiative has provided valuable insight for the development and optimization of III-V nitride optoelectronic devices, particularly, blue/UV quantum well lasers.

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PROJECT SUMMARY

Two main objectives of this research program include: (1) investigation of the fundamental material, transport, and optical properties of III-V nitrides; and (2) simulation and design optimization of GaN-based optoelectronic devices. Study of fundamental physical properties (such as carrier scattering and optical transitions) is based on an envelope function formalism for accurate description of band spectrum in bulk and confined structures. Numerical analyses and optimization of GaN-based devices are approached by solving a set of coupled equations self-consistently. This research initiative has provided valuable insight for the development and optimization of III-V nitride optoelectronic devices, particularly, blue/UV quantum well lasers.

SUMMARY OF RESEARCH PROGRESS

During the project period, we developed an envelope function formalism for band spectrum in bulk wurtzite semiconductors and quantum wells; extracted a set of material (including strain-related) parameters for GaN-based structures; derived a unified approach for optical transitions between valence and conduction bands (including intervalence band transitions); and obtained results on hole-phonon scattering and transport characteristics in GaN. Furthermore, coupled Poisson-Schrödinger equations were solved self-consistently under the envelope function formalism and the effects of strain and piezoelectric field on optical gain were studied in GaN quantum well laser structures. A brief description of each result is given below. More details can be found in our publications whose list is provided at the end of this section.

- An envelope function formalism for the valence band spectrum of wurtzite structures was developed starting from the Rashba-Sheka-Pikus Hamiltonian for coupled Γ_9, Γ_7, and Γ_7 levels. A cubic approximation has been derived for 10 (16 in the presence of strain) material constants for hole band structure, and the commonly used notation of Bir and Pikus has been corrected. The concept of wurtzite as a prestrained cubic material was introduced quantitatively by deriving a relationship between the hexagonal crystal field splitting and the equivalent additional biaxial strain components.
- The valence band parameters of wurtzite GaN were estimated by matching the results of existing ab initio energy band calculations with analytical expressions of the envelope-function formalism. In addition, deformation potentials and splitting energies for GaN were determined by nonlinear fitting to the experimental results. The calculated A-, B-, and C-type hole dispersion relations show strongly anisotropic characteristics and anti-crossing features in energy spectrum due to band mixing effects.
- Valence band structures in pseudomorphically strained quantum wells have been obtained by constructing an analytical solution and/or purely numerical calculations. Results of both approaches are in perfect agreement with each other providing a validation for both methods of calculations. A detailed analysis was conducted for the dependence of hole spectrum on quantum well width, depth, and strain due to lattice mismatch.
- Matrix elements for optical transitions from the conduction band to the valence bands as well as between valence bands (i.e., intervalence band) have been derived analytically. Dependence of the transition matrix element on the emitted light polarization and/or strain was analyzed in detail and interpreted based on the symmetry properties of carrier Bloch states in wurtzite-type crystals. Furthermore, calculations have been conducted for optical gain in both bulk and GaN-based quantum wells. Unlike the unstrained cubic materials, the optical gain in bulk wurtzite GaN exhibits a strong polarization dependence. For a given carrier concentration, the peak gain is the largest

when the electric field is perpendicular to the c axis. The calculated transparency concentration is consistent with the experimental data.

- Electron transport properties have been described for GaN in bulk and quantum wells. First, ensemble Monte Carlo calculations of steady-state electron drift velocity were obtained as a function of the applied electric field. Transient transport was also studied to examine the role of ballistic electron effects. We demonstrated that in most cases, electrons in GaN lose their directed average velocity over distances of only 10–20 nm, and ballistic transport occurs only within such short distances.
- Hole scattering was treated using an accurate description of the valence band states in wurtzite-type structures. In particular, analytical expressions for the Bloch overlap factors (describing hole scattering by Coulomb impurities and polar optical phonons) have been derived. Dependence of the scattering matrix elements on wave vector direction and/or applied strain has been discussed and compared to the similar values in cubic structures. It has been demonstrated that compared to the cubic symmetry, an additional anisotropy appears in hexagonal crystals due to the existence of a preferential direction (c-axis).
- A self-consistent calculation of optical gain and the corresponding differential gain was performed for pseudomorphically strained GaN quantum wells as a function of carrier density. Based on the local exchange-correlation potential, electron and hole band structures were obtained by coupling Poisson's equation with an effective-mass Schrödinger equation in the conduction band and an envelope-function Hamiltonian in the valence band. Our calculations show that self-consistent calculations including the piezoelectric effects are essential for accurate description of strained wurtzite quantum-well structures.

REFEREED PUBLICATIONS

During the contract period, this program has resulted in six refereed publications in the literature. Reprints of these publications supported by ARO have been sent to the program manager under separate cover:

Y. M. Sirenko, J.-B. Jeon, K. W. Kim, M. A. Littlejohn, and M. A. Stroscio, "Envelope-Function Formalism for Valence Bands in Wurtzite Quantum Wells," *Phys. Rev. B* 53, 1997 (1996).

J.-B. Jeon, Y. M. Sirenko, K. W. Kim, M. A. Littlejohn, and M. A. Stroscio, "Valence Band Parameters of Wurtzite Materials," *Solid State Commun.* 99, 423 (1996).

Y. M. Sirenko, J.-B. Jeon, K. W. Kim, M. A. Littlejohn, and M. A. Stroscio, "Strain Effects on Valence Band Structure in Wurtzite GaN Quantum Wells," *Appl. Phys. Lett.* 69, 2504 (1996).

N. S. Mansour, K. W. Kim, N. A. Bannov, and M. A. Littlejohn, "Transient Ballistic Transport in GaN," *J. Appl. Phys.* 81, 2901 (1997).

B. C. Lee, N. S. Mansour, Y. M. Sirenko, K. W. Kim, and M. A. Littlejohn, "Anisotropic Hole Scattering in Hexagonal GaN," *Semicond. Sci. Technol.* 12, 280 (1997).

J. Wang, J. B. Jeon, Y. M. Sirenko, and K. W. Kim, "Piezoelectric Effect on Optical Properties of Pseudomorphically Strained Wurtzite GaN Quantum Wells," *IEEE Photon. Technol. Lett.* 9, 728 (1997).